201-15143

IUCLID

Data Set

Robust Summaries

Existing Chemical	:	ID: 80-51-3
CAS No.	:	80-51-3
EINECS Name	:	Benzenesulfonic acid, 4,4'-oxybis-, dihydrazide
EC No.	:	201-286-1
Molecular Formula	:	C12H14N4O5S2
Status	:	
Memo	:	Celogen OT Crompton US HPV
Printing date	:	23.06.2003
Revision date	:	
Date of last update	:	23.06.2003
Number of pages	:	14
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

2.1 MELTING POINT

Decomposition	:	yes, at 150 - 160 °C
Test substance	:	Benzenesulfonic acid, 4,4'-oxybis-, dihydrazide (CAS No. 80-51-3)
Reliability	:	(1) valid without restriction Peer reviewed literature

17.03.2003 (3)

2.2 BOILING POINT

Decomposition	:	yes
Year	:	
GLP	:	
Test substance	:	Benzenesulfonic acid, 4,4'-oxybis-, dihydrazide (CAS No. 80-51-3)
Remark	:	Decomposes prior to melting

17.03.2003 (3)

2.4 VAPOUR PRESSURE

Value	:	.0000000000089 hPa at 25 °C
Decomposition	:	
Method	:	other (calculated): MPBPWIN v1.40
Year	:	2003
GLP	:	
Test substance	:	Benzenesulfonic acid, 4,4'-oxybis-, dihydrazide (CAS No. 80-51-3)

26.03.2003 (6)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	octanol-water
Log pow	:	.08 at °C
pH value	:	
Method	:	other (calculated): KOWWIN v1.66
Year	:	2003
GLP	:	
Test substance	:	Benzenesulfonic acid, 4,4'-oxybis-, dihydrazide (CAS No. 80-51-3)
Reliability	:	(2) valid with restrictions

26.03.2003 (6)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	4733 mg/l at °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	

Method	:	other: Calculated using WSKOW v1.40
Year	:	
GLP	:	
Test substance	:	Benzenesulfonic acid, 4,4'-oxybis-, dihydrazide (CAS No. 80-51-3)
Reliability	:	(2) valid with restrictions

26.03.2003 (6)

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
INDIRECT PHOTOLYSIS		
Halflife t1/2	:	61 hour(s)
Degradation	:	% after
Quantum yield	:	
Deg. product	:	
Method	:	other (calculated): AOPWIN v1.90
Year	:	2003
GLP	:	
Test substance	:	
Remark	:	Concentration of hydroxyl radicals in air = 1.5E6 OH/cm3 12-hour day
Test substance	:	Benzenesulfonic acid, 4,4'-oxybis-, dihydrazide (CAS No. 80-51-3)
Reliability	:	(2) valid with restrictions

26.03.2003 (6)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	fugacity model level III
Media	:	
Air	:	% (Fugacity Model Level I)
Water	:	% (Fugacity Model Level I)
Soil	:	% (Fugacity Model Level I)
Biota	:	% (Fugacity Model Level II/III)
Soil	:	% (Fugacity Model Level II/III)
Method	:	other: calculation using Epiwin Level III Fugacity Model
Year	:	2003
Test condition	:	Henry's Law Constant: 1.26E-17 atm-m3/mole (Henrywin program) Vapor pressure: 6.67E-12 mmHg (Mpbpwin program) Log Kow: 0.08 (KOWWIN program) Soil Koc: 0.493 (calc by model) Melting point: 237 °C (MpBpwin program) 1000 kg/hr emissions to air, water and soil compartments.
Test substance	:	Benzenesulfonic acid, 4,4'-oxybis-, dihydrazide (CAS No. 80-51-3)
Attached document	:	Fugacity Model Data.doc

	Mass Amount (percent)	Half-life (hr)	Emissions (kg/hr)
Air	2.35E-7	122	1000
Water	49.1	900	1000

Soil	50.8	900	1000
Sediment	0.0916	3.6E+3	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	3.52E-21	3.17E-5	5.59E-5	1.06E-6	1.86E-6
Water	2.05E-22	900	1.17E+3	30	39
Soil	7.57E-21	931	0	31	0
Sediment	1.89E-22	0.42	0.0436	0.014	0.00145

Persistence time: 793 hr
Reaction time: 1.3E+3 hr
Advection time: 2.04E+3 hr
Percent reacted: 61
Percent advected: 39

Half-lives (hr), (based upon Biowin (ultimate) and Aopwin):
Air: 122
Water: 900
Soil: 900
Sediment: 3600
Biowin estimate: 2.349 (weeks-months)

Advection times (hr):
Air: 100
Water: 1000
Sediment: 5E+4

Reliability : (1) valid without restriction
26.03.2003 (6)

3.5 BIODEGRADATION

Type : Aerobic
Inoculum :
Deg. product :
Method : other: Estimation using BIOWIN v4.00
Year : 2003
GLP :
Test substance : Benzenesulfonic acid, 4,4'-oxybis-, dihydrazide (CAS No. 80-51-3)
Result : MITI linear biodegradation probability = -0.466
MITI non-linear bidegradation probability = 0.000

Not Readily biodegradable
Reliability : (2) valid with restrictions
26.03.2003 (6)

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	
Species	:	
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	9.76
Method	:	other: calculation using Ecosar v0.99g
Year	:	2003
GLP	:	
Test substance	:	Benzenesulfonic acid, 4,4'-oxybis-, dihydrazide (CAS No. 80-51-3)
Test condition	:	Log Kow: 0.08 (KowWin estimate) Water solubility: 1.45E+5 (calculated) Ecosar class: Hydrazines
Reliability	:	(2) valid with restrictions

26.03.2003 (6)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	
Species	:	Daphnia sp. (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
EC50	:	17.37
Method	:	other: calculation using Ecosar v0.99g
Year	:	2003
GLP	:	
Test substance	:	Benzenesulfonic acid, 4,4'-oxybis-, dihydrazide (CAS No. 80-51-3)
Test condition	:	Log Kow: 0.08 (KowWin estimate) Water solubility: 1.45E+5 (calculated) Ecosar class: Hydrazines
Reliability	:	(2) valid with restrictions

26.03.2003 (6)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	:	
Endpoint	:	
Exposure period	:	144 hour(s)
Unit	:	mg/l
EC50	:	2.36
Method	:	other: calculation using Ecosar v0.99g
Year	:	2003
GLP	:	
Test substance	:	Benzenesulfonic acid, 4,4'-oxybis-, dihydrazide (CAS No. 80-51-3)
Test condition	:	Log Kow: 0.08 (KowWin estimate) Water solubility: 1.45E+5 (calculated) Ecosar class: Hydrazines
Reliability	:	(2) valid with restrictions

26.03.2003 (6)

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	> 5200 mg/kg bw
Species	:	rat
Strain	:	other: albino
Sex	:	no data
Number of animals	:	
Vehicle	:	other: olive oil
Doses	:	Maximum dose was 9 cc of a 14.3% solution
Method	:	other: United States Testing Co., Inc method
Year	:	1950
GLP	:	no
Test substance	:	Benzenesulfonic acid, 4,4'-oxybis-, dihydrazide (CAS No. 80-51-3) Supplier: Naugatuck Chemical Co. Lot No: ILGE A-2609 Purity: No data
Method	:	Post dose observation period: 3 days
Result	:	The minimum oral LD50 of a compound is the minimum dose which may be expected to kill half of the animals in a test group upon oral administration. In this study, an oral LD50 was not obtainable at the highest level fed. The highest level fed was equivalent to 1.3g of the sample for rats weighing approximately 250 g, i.e. 5200 mg/kg.
Reliability	:	(2) valid with restrictions

27.03.2003 (5)

Type	:	LD50
Value	:	2300 mg/kg bw
Species	:	Rat
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Method	:	Unknown
Year	:	2002
GLP	:	
Test substance	:	Benzenesulfonic acid, 4,4'-oxybis-, dihydrazide (CAS No. 80-51-3) Purity: No data
Reliability	:	(4) not assignable

23.06.2003 (7)

5.1.3 ACUTE DERMAL TOXICITY

Type	:	
Value	:	
Species	:	Rabbit
Strain	:	

Sex	:	
Number of animals	:	10
Vehicle	:	Water
Doses	:	200 mg/kg
Method	:	other: FIFRA Section 162.8 (c), March 1948
Year	:	1950
GLP	:	No
Test substance	:	Benzenesulfonic acid, 4,4'-oxybis-, dihydrazide (CAS No. 80-51-3) Supplier: Naugatuck Chemical Co. Lot No: ILGE A-2609 Purity: No data
Method	:	The calculated dosage was first dissolved in distilled water and then placed onto gauze squares. The squares were immediately placed on the bare skin of each rabbit and securely held in place with waterproof adhesive tape. Care was taken to completely cover each patch securely so as to minimize evaporation and to insure continuous contact with the skin for 24 hours.
Result	:	The following observations were made after 24 hours: 1. All animals were alive and well after the 24 hour period 2. No toxic manifestations were exhibited by any of the animals under test.
Reliability	:	(2) valid with restrictions

27.03.2003 (5)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

Type	:	LD50
Value	:	> 5000 mg/kg bw
Species	:	Mouse
Strain	:	
Sex	:	no data
Number of animals	:	
Vehicle	:	physiol. Saline
Doses	:	up to 2.5 c.c. of a 5% solution
Route of admin.	:	i.p.
Exposure time	:	
Method	:	other: United States Testing Co., Inc method
Year	:	1950
GLP	:	No
Test substance	:	Benzenesulfonic acid, 4,4'-oxybis-, dihydrazide (CAS No. 80-51-3) Supplier: Naugatuck Chemical Co. Lot No: ILGE A-2609 Purity: No data
Method	:	Post dose observation period: 3 days
Result	:	Unable to obtain a definite killing point. The highest concentration injected was equivalent to 5000 mg/kg b.w.
Reliability	:	(4) not assignable

27.03.2003 (5)

5.2.1 SKIN IRRITATION

Species	:	Rabbit
Concentration	:	50 mg
Exposure	:	
Exposure time	:	24 hours
Number of animals	:	
Vehicle	:	Other
PDII	:	
Result	:	
Classification	:	
Method	:	EPA OPP 81-5
Year	:	1950
GLP	:	No
Test substance	:	As prescribed by 1.1-1.4
Method	:	50 mg of the sample was mixed with Vaseline and placed on to gauze squares, which were then placed on the bare skin of rabbits. The squares were held in place by waterproof adhesive tape. This test was conducted on 3 rabbits. As a control the effect of pure Vaseline was tested in a similar manner. The patches were removed 24 hours later and the skin was observed for signs of irritation
Result	:	Slight reaction was observed in the treated rabbits and there was no irritation seen in the control
Reliability	:	(4) not assignable

23.07.2003 (7)

Species	:	rabbit
Concentration	:	
Exposure	:	
Exposure time	:	
Number of animals	:	3
Vehicle	:	physiol. saline
PDII	:	
Result	:	
Classification	:	
Method	:	other: United States Testing Co., Inc method
Year	:	1950
GLP	:	No
Test substance	:	Benzenesulfonic acid, 4,4'-oxybis-, dihydrazide (CAS No. 80-51-3) Supplier: Naugatuck Chemical Co. Lot No: ILGE A-2609 Purity: No data
Method	:	The test substance was extracted in 5% amounts in physiological saline in an autoclave. The extracts were then injected with aseptic precautions into the rabbits. Ater 24 hours the rabbits were observed for presence of irritation.
Result	:	There was a slight reaction caused by the extracts of the sample.
Reliability	:	(4) not assignable

27.03.2003 (5)

5.4 REPEATED DOSE TOXICITY

Type	:	
Species	:	Rat
Sex	:	male/female
Strain	:	
Route of admin.	:	oral feed
Exposure period	:	90 days
Frequency of treatm.	:	Daily
Post exposure period	:	
Doses	:	20 ppm (1mg/kg bw/day), 2000 ppm (100 mg/kg bw/day)
Control group	:	
Method	:	
Year	:	1981
GLP	:	
Test substance	:	Benzenesulfonic acid, 4,4'-oxybis-, dihydrazide (CAS No. 80-51-3)
Remark	:	This study is limited because a restricted range of tissues of only half of any group of treated animals were subject to detailed microscopic examination.
Result	:	NOEL = 1 mg/kg bw/day Groups of 12 rats of each sex fed diets containing 2000 ppm (100 mg/kg bw/day) for 90 days showed reduced food consumption and depressed growth, and two of the male rats died within 10 weeks appearing malnourished. Increased liver and kidney weights were noted, but no macroscopic abnormalities or effects on the blood were seen in the surviving animals. These findings were attributed by the investigators to the low palatability of the diet. No effects were observed in animals fed 20 ppm (1 mg/kg bw/day).
Reliability	:	(4) not assignable

16.05.2003 (1)

Type	:	
Species	:	Rat
Sex	:	
Strain	:	
Route of admin.	:	Gavage
Exposure period	:	4 months
Frequency of treatm.	:	Daily
Post exposure period	:	
Doses	:	
Control group	:	
LOAEL	:	36 mg/kg bw
Method	:	
Year	:	1969
GLP	:	
Test substance	:	Benzenesulfonic acid, 4,4'-oxybis-, dihydrazide (CAS No. 80-51-3)
Result	:	Doses of approximately 200 mg/kg bw/day by stomach tube killed all six rats within 2 weeks. Growth was reduced in six rats given 36 mg/kg bw/day by stomach tube for 4 months. Increased liver weight, disturbance of liver and kidney function and changes in the appearance of the liver, kidney and adrenals were also seen.
Reliability	:	(4) not assignable

16.05.2003 (4)

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	Chromosome aberration test
System of testing	:	
Test concentration	:	
Cycotoxic concentr.	:	
Metabolic activation	:	
Result	:	Negative The results indicate that the test substance did not cause a statistically significant increase in the number of chromosome aberrations ($p<0.05$). This was observed for both activated and non-activated systems. In addition, there was no detectable dose response in the number of aberrations of both activated and non-activated systems, verifying the validity of the test system. In conclusion, the test substance did not induce chromosomal aberrations in Primary Cultured Human Lymphocytes and is considered non-clastogenic
Method	:	The test substance was evaluated for its ability to induce chromosomal aberrations in primary human lymphocyte cells in the presence and absence of a rat liver homogenate metabolic activation system. The test article was tested at the following concentrations: Neat and 1:2, 1:4, 1:8, 1:16, 1:32 and 1:64 dilutions of the neat extract. The concentrations chosen to be scored for the activated assay were Neat and 1:2 and 1:4 dilutions of the test extract. The following controls were used: 1. Negative Control Article:- RPMI Cell Culture medium, the extraction vehicle, served as the negative control article. 2. Positive Control Article (Non-activated system):- Mitomycin C (MMC) is a known mutagen and clastogenic agent and served as the positive control article for the non activation system. 3. Positive Control Article (Activated System):- Cyclophosphamide (CP) is a clastogen that requires metabolic transformation by microsomal enzymes. It served as the positive control article for the activation assay
Year	:	1997
GLP	:	
Test substance	:	Benzenesulfonic acid, 4,4'-oxybis-, dihydrazide (CAS No. 80-51-3) Purity: no data
Reliability	:	(4) not assignable

23.06.2003 (7)

Type	:	Bacterial reverse mutation assay
System of testing	:	
Test concentration	:	Neat, 1:2, 1:4, 1:8 and 1:20 fold dilutions.
Cycotoxic concentr.	:	
Metabolic activation	:	+/-
Result	:	Positive
Method	:	EPA OTS 798.5265
Year	:	1997
GLP	:	Yes
Test substance	:	Benzenesulfonic acid, 4,4'-oxybis-, dihydrazide (CAS No. 80-51-3) Purity: no data

Method	:	The Salmonella typhimurium Reverse Mutation Assay (Ames Assay) test was conducted to evaluate the potential for the test substance to induce histidine reversion caused by base changes or frameshift mutations in the genome of this organism. The direct plate incorporation assay was conducted with four strains of Salmonella typhimurium in the presence and absence of exogenous mammalian activation system.
Result	:	The test substance is mutagenic.
Reliability	:	(4) not assignable

23.06.2003 (7)

Type	:	Bacterial reverse mutation assay
System of testing	:	
Test concentration	:	
Cycotoxic concentr.	:	
Metabolic activation	:	
Result	:	Positive
Method	:	
Year	:	
GLP	:	
Test substance	:	Benzenesulfonic acid, 4,4'-oxybis-, dihydrazide (CAS No. 80-51-3) Purity: no data
Remark	:	Benzenesulfonic acid, 4,4'-oxybis-, dihydrazide was mutagenic in Salmonella typhimurium (Ames test) in the presence or absence of a liver metabolic activation system (Hachiya, 1987; Shimizu, 1986; Shimizu et al, 1978). In a test with one strain of Escherichia coli, a liver metabolic activation system was required for the hydrazide to exhibit mutagenic potential (Shimizu, 1986), although tests with other strains (Hachiya, 1987; Shimizu, 1986), found no evidence of mutagenicty in the presence or absence of a liver metabolic fraction.
Reliability	:	(4) not assignable

16.05.2003 (2)

5.6 GENETIC TOXICITY 'IN VIVO'

Type	:	Micronucleus assay
Species	:	
Sex	:	
Strain	:	
Route of admin.	:	
Exposure period	:	
Doses	:	
Result	:	Negative
Method	:	
Year	:	
GLP	:	
Test substance	:	Benzenesulfonic acid, 4,4'-oxybis-, dihydrazide (CAS No. 80-51-3) Purity: no data
Reliability	:	(4) not assignable

23.06.2003 (7)

Type	:	Unscheduled DNA synthesis
Species	:	
Sex	:	
Strain	:	
Route of admin.	:	
Exposure period	:	
Doses	:	
Result	:	Negative
Method	:	
Year	:	
GLP	:	
Test substance	:	Benzenesulfonic acid, 4,4'-oxybis-, dihydrazide (CAS No. 80-51-3) Purity: no data
Reliability 23.06.2003	:	(4) not assignable (7)

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

(1) Borgstedt, H.H. (1981). 90-day feeding study in rats. Final report volume 1. Department of Pharmacology & Toxicology. University of Rochester. USA; reported in BIBRA International Ltd (1997). Toxicity Profile for 4,4'-Oxybis(benzenesulphonylhydrazide)

(2) Hachiya, N. (1987). Akita J. Med. 14 269; Shimizu, H. (1986). Tokyo Jikeika med. J. 101, 167; Shimizu, H. et al (1978)Jpn J. Hygiene 33, 474; reported in BIBRA International Ltd (1997). Toxicity Profile for 4,4'-Oxybis(benzenesulphonylhydrazide)

(3) Hawley, G.G., The Condensed Chemical Dictionary, 9th ed., New York, Nostrand Rheinhold Co., p 643, 1977

(4) Shurupova, G.A., et al (1969). Sin. Issled Eff. Khimikatov. Polim. Mater. 3, 438; reported in BIBRA International Ltd (1997). Toxicity Profile for 4,4'-Oxybis(benzenesulphonylhydrazide)

(5) United States Testing Company, Inc, Test Report 21672, July 21, 1950

(6) US EPA, EPIWIN v3.10, EPI Suite Software, 2000

(7) IUCLID Dataset for Existing Chemicals, 4, 4'-oxydi(benzenesulfonohydrazide), 2002